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The maximum entropy principle and Schrödinger eigenvalue problems

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Abstract The possibility of employing the maximum entropy principle, without any *a priori* knowledge of moments, to construct approximate density functions for bound, stationary quantum states has been explored. A viable scheme based on the fusion of the prescription provided by the above principle, with modifications as and when necessary, and the Rayleigh-Ritz variational approach has been put forward. Both ground and excited states of several problems in $[-\infty, \infty]$ are considered. The extension to problems with finite boundaries has also been investigated. Pilot calculations involving various anharmonic oscillators, the particle-in-a-box and its supersymmetric partner demonstrate the success of the endeavour beyond any doubt.

Keywords Maximum entropy principle, variational method, bound-state calculations

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1. Introduction

Given as input a set of moments μ_n $(n \le k)$ of a variable x in $[a, b]$ corresponding to an exact probability density (PD) $P(x)$, where

$$\mu_n = \langle x^n \rangle = \int x^n P(x)\,dx, \quad n = 0, 1, 2, \ldots, k, \quad (1)$$

the maximum entropy principle (MEP) [1] advocates maximization of the information entropy functional $I[P]$ given by

$$I[P] = -\int P(x)\ln[P(x)]\,dx \quad (2)$$

to find $P(x)$, subject to the constraints imposed by (1). By standard manipulations, one obtains the following form of an approximate density $P^A(k, x)$:

$$P^A(k,x) = \exp\left(-S^A(k,x)\right) = \exp\left(-\sum_{n=0}^{k}\lambda_n x^n\right). \quad (3)$$

This MEP recipe is known [2] to provide the *least biased* estimate of the PD consistent with the available information. Plastino and coworkers [3] have made nice use of it in stationary quantum mechanics to obtain good approximations to ground-state eigenvalues and eigenfunctions of Hamiltonians that are not exactly solvable. The extension to the many-body context by these authors [4] has also been found encouraging. However, the approach requires values of the first few moments.

Problems inherent in the above procedure are the following : (A) Except for some special circumstances where certain moments are experimentally obtained, use of (3) in (1) to get $\{\lambda_n\}$ presupposes values for moments derived from other theoretical sources. This means that the problem has already been solved somehow. The present scheme thus loses generality. (B) The MEP prescription (3) tells us that the PD should go as $\exp(-\lambda_k x^k)$ at large x. The asymptotic behaviour of $P^A(k, x)$ is thus *dictated* by the *number* of moments employed to *construct* it. This is highly undesirable. For a given problem, $P(x)$ should have a *unique* asymptotic fall-off. (C) If we choose a one-dimensional problem with a real potential, the approximate wavefunction may then be written as

$$\psi^A(k,x) = [P^A(k,x)]^{1/2}. \quad (4)$$

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Table 1. Ground state energies for potentials in (8) *via* VMEP using the PD (7).

Case	Potential parameters				k	E_0
	α	β	γ	δ		
1	0	1	0	0	1	1 08
					2	1 0604
					3	1 0604
					4	1 0603622
						(1 06036209)[a]
2	0	40000	0	0	1	36 99
					2	36 267
					3	36 267
					4	36 2662
						(36 263873)[a]
3	1	1	0	0	1	1 40
					2	1 39238
					3	1 39238
					4	1 39235166
						(1.392351642)[a]
4	1	40000	0	0	1	37 0
					2	36 277
					3	36 277
						(36 274458)[a]
5	1	1	0	0	1	0 70
					2	0 658
					3	0 658
					4	0 6576538
						(0 6576530)[b]
6	0	0	1	0	1	1 22
					2	1 145
					3	1 14482
					4	1 14482
					5	1 14480248
						(1 144802454)[a]

[a]See Ref [10]. [b]See Ref [11]

It is mandatory for $\psi(x)$ to vanish at the boundaries. This feature should be embedded in $P^A(k, x)$. When $x \in [-\infty, \infty]$, it may be ensured by requiring the sign of λ_k in $S^A(k, x)$ to be positive. But, if the actual $P(x)$ goes to zero at one or more points within the said interval, form (3) of $P^A(k, x)$ becomes inadequate. This at once negates the possibility of a straightforward implementation of the MEP to excited bound states. For $x \in [a, b]$ the difficulty is worse. In this case, even the ground state is not amenable to a standard MEP treatment since the form (3) cannot vanish at finite boundaries. Understandably, then, work referred to above [3] has concentrated only on *ground* states in $[-\infty, \infty]$ So one wonders how one would modulate the MEP form (3) to make it applicable to these other situations. (D) Without any *a priori* knowledge of moments, bare maximization of $I[P^A(k, x)]$ does not yield properly optimized PD. This is because no information regarding the potential is incorporated. One may be tempted to introduce this information in a rough manner through the use of the virial theorem (VT) [5] as a constraint in the optimization process. But our numerical experience tells that this is not enough. The reason is : a multivariate function like (3) obeys the VT over various ranges in the parameter space. Moreover, the VT is necessary but *not* a sufficient criterion for a wavefunction to be accurate. As an alternative, one could think of utilizing the far more stringent criterion of the constancy of local energy [6]; but, it does not easily fit into the MEP framework. So, we have to seek some other route to employ the MEP form of PD if we wish to bypass (1).

Having discussed the subtleties of the MEP approach with reference to its application to bound quantum states, the purpose of the present communication is to put forward a variational recipe that does not require any *a priori* knowledge of moments but still uses the basic spirit of MEP. Thus, we avoid problems A and D. A variational formulation [7] of the problem allows us to employ $P^A(k, x)$ in (3) as a *trial* density, containing $(k + 1)$ parameters, to be optimized Treating $S^A(k, x)$ in (3) as a *function* that admits a series expansion, we shall see that problem B can also be overcome [8] Finally, a suitable prefactor [8] can handle cases in finite intervals, while a linear variational strategy [9] with a specific, derived set of orthogonal polynomials, to be discussed below, will be found to efficiently deal with PD with nodes. Thus, problem C can also be avoided.

Our work is organized as follows. First, in Section 2, we recast the primitive MEP ansatz in variational mould. This will enable us to treat $\{\lambda_m\}$ in (3) as variational parameters rather than as Lagrange multipliers incorporating constraint relations (1). Next we show that, unless the large-x behaviour of $P^A(k, x)$ is properly built into the MEP ansatz, results are not sensitive enough. We then propose a way of modifying the prevalent MEP ansatz (3) for the PD. Section 3 is devoted to studies on excited states where a coupled variational approach is adopted to compute the first N excited states of a system in one stroke. For this purpose we invoke a set of orthogonal polynomials with the ground state density as the weight function. This procedure broadens the scope of our variational MEP (VMEP) approach. In Section 4, we concern ourselves with the ground and excited states of quantum mechanical problems where the PD vanishes at finite boundaries.

Pilot calculations in this work involve various anharmonic oscillators, the problem of a particle-in-a-box (PB) and its supersymmetric (SUSY) partner. The reason for choosing these simple energy eigenvalue problems, where near-exact results are available through a variety of routes [10, 11], is to provide a reliable yardstick for assessing the strength of our approach.

As regards the numerical work involved in this paper, we have relied mainly upon the conjugate gradient method of

owell as discussed in Ref. [12]. A more direct method based n random variations of the parameters as outlined by illingbeck [13] has also been employed by us occasionally quicken the optimization process as well as to provide a oss-check.

Variational MEP for ground states in $[-\infty, \infty]$

et us consider a positive semidefinite, real potential $V(x)$ at satisfies $V(x) = V(-x)$. This dictates $P(x) = P(-x)$, and r bound states, we further require that $P(x)$ is normalizable. Vithout any loss of generality one can choose

$$\int_{-\infty}^{\infty} P(x)dx = 1. \tag{5}$$

hese considerations also apply to $P^A(k, x)$. Given the amiltonian

$$H = \frac{d^2}{dx^2} + V(x), \tag{6}$$

e odd moments naturally disappear. Thus, if we had owledge of the even moments μ_2, μ_4, *etc.*, we might nstruct an unnormalized PD

$$P^A(k,x) = \exp\left(-S^A(k,x)\right) = \exp\left(-\sum_{n=1}^{\infty} \lambda_{2n} x^{2n}\right) \tag{7}$$

he natural choice now is to treat the form (7) as a *trial ensity* and use the standard Rayleigh-Ritz variational rinciple This does not require any added constraint. One n also clearly judge the efficacy of form (7) for density nd think of possible improvements. The parameters in (7) e determined by minimizing the ground state energy E_g. Ve choose the following general form for $V(x)$:

$$V(x) = \alpha x^2 + \beta x^4 + \gamma x^6 + \delta x^8. \tag{8}$$

ample results are presented in Table 1. We show here the ffect of gradually increasing the number of terms in $S^A(k, x)$ n the average ground state energy E_g. This tests directly the ptness of the primitive MEP ansatz. For comparison, the xact result in each case is shown in parentheses. For brevity, e choose presently $\delta = 0$ in (8).

Let us note a few points now. Usually, there is a gradual nprovement in the results as we increase the number of arameters, which is expected. But, in some cases, results o not improve *at all* even when one *extra* variational arameter is embedded in $P^A(\lambda, x)$. This is a disturbing eature that requires a closer scrutiny. To this end, let us put $^A(k, x)$ given by (7) in the energy eigenvalue equation here $V(x)$ has the form (8). Equating the coefficients of ven powers of x on both sides we obtain

$$\sum_{ij} 4ij\lambda_{2i}\lambda_{2j}x^{2i+2j-2} - \sum_{i} i(2i-1)\lambda_{2i}x^{2i-2} = \left(\alpha x^2 + \beta x^4 + \gamma x^6 - E_g\right) \tag{9}$$

From this relation we can express λ_{2n} in terms of E_g. By using a reasonably accurate value of E_g, it can be checked that the sign of λ_6 is negative in cases 1 to 5 in Table 1, and in case 6 the parameter λ_8 is so. Thus the use of $P^A(k, x)$, truncated at $k = 3$ and hence requiring a positive λ_6 for normalizability in cases 1 to 5, cannot improve results. A similar situation arises for λ_8 in case 6. In these cases, energy minimization is achieved by taking the parameters corresponding to the highest power of x very small and positive ($\approx 10^{-8}$) leading to results no better than those with one parameter less.

It appears that efforts aimed at further improvement of results by increasing the degree of the polynomial $S^A(k, x)$ will be *unwise* on two counts : (i) the non-linear optimization procedure becomes messy and (ii) the corresponding form for $P^A(k, x)$ increasingly departs from the true asymptotic behaviour for the given potential. For example, if $V(x) = \gamma x^6$, one expects a fall-off of density as $\exp(-x^4)$. On the other hand, in Table 1, we have achieved the maximum energy lowering *already* at the cost of a fall-off going as $\exp(-x^{10})$ in this case (*cf.* case 6). Naturally, further improvement in energy by gradually increasing the number of parameters in the manner sketched above should lead only to a worsening of the asymptotic behaviour. The moral then is : this procedure cannot take us to exactness. For the quartic problem, the situation is more disturbing because here the density should decay as $\exp(-|x^3|)$ whereas $S^A(k, x)$ is an even polynomial. This feature of the quartic oscillator problem has been noted earlier [14,15], albeit in different contexts. All these considerations prompt us to seek a modified strategy in the VMEP framework.

The modification is achieved by treating the series $S^A(k, x)$ as a function that respects

$$P^A(k,x) \sim \exp(-x^4), |x| \to \infty, \tag{10}$$

for $\delta = 0$, $\gamma \neq 0$ in (8) A very convenient way to meet this requirement is provided by Pade' approximants (PA) [16]. The simplest choice would thus be

$$S^A(x) = \frac{p_1 x^2 + p_2 x^4 + p_3 x^6}{1 + q_1 x^2}. \tag{11}$$

And here we see that $S^A(x)$ is really a *function* that admits of a series representation. The general structure of $S^A(k, x)$ in this scheme will be

$$S^A(k,x) = \frac{p^A_{k/2+1}(x^2)}{q^A_{k/2-1}(x^2)} \tag{12}$$

which is a $[M, M\text{-}2]$ type PA, except for the constant term in the numerator that is here absorbed in normalization. We can thus generate a family of trial densities by varying k in this case. But, this strategy cannot be applied to $V(x)$ in (8) with $\delta = \gamma = 0$ for obvious reasons. We have to choose a more general form of $S^A(k, x)$. This form reads as

$$S^A(k,x) = \frac{\left[p^A_r(x^2)\right]^s}{\left[q^A_t(x^2)\right]^u} \equiv [r, s/t, u], \tag{13}$$

where r, s, t and u are judiciously chosen to satisfy the asymptotic behaviour for a given potential problem. The highest power of x in polynomial p_r^A is $2r$ whereas in q_t^A it is $2t$. The constant term in the former is taken as zero while in the latter it is unity. The true density goes as $\exp(-x^2)$ as $x \to 0$ in all the cases. We set $s = 1$ in (13) to respect this behaviour. The total number of unknown parameters in the PD is then $k = (r + t)$. In Table 2, we display some results following this modification, corresponding to cases discussed in Table 1.

Table 2. Ground state energies for potentials in (8) *via* an improved VMEP employing the power-Padé form (13) in (7)

Case	r	t	u	E_g
1	2	1	1/2	1.060362093
	2	2	1/4	1.0603620920
	3	3	1/2	1.06036209050
	2	4	1/8	1.06036209049
				(1.06036209048)[a]
2	2	1	1/2	36.26387349
	2	2	1/4	36.26387344
	2	4	1/8	36.26387338993
				(36.263873389915)[a]
3	2	1	1/2	1.39235164160
	2	2	1/4	1.39235164154
	2	4	1/8	1.3923516415304
				(1.3923516415303)[a]
4	2	1	1/2	36.27445823
	2	2	1/4	36.27445819
	2	4	1/8	36.27445813375
				(36.274458133737)[a]
5	2	1	1/2	0.657653039
	2	2	1/4	0.657653006
	2	4	1/8	0.65765300051862
				(0.65765300051856)[b]
6	3	1	1	1.14480246
	4	2	1	1.144802454
				(1.1448024538)[a]

[a]See Ref. [10], [b]See Ref. [11]

Comparing these results with the earlier ones, it is quite clear that if the trial PD conforms to the *correct* asymptotic behaviour, there is a *significant* improvement in the energies and hence in the quality of the density. Thus, by clinging to power-Padé type approximants (13), a nicely workable functional form of $S^A(k, x)$ may be constructed if only the small- and large-x behaviours of the density are known *a priori*.

3. Variational MEP for excited states in $|-\infty, \infty|$

We now discuss how our formalism can be extended to deal with excited states. The PD given by (3) can vanish only at $x = \pm\infty$, but does not support nodes at any finite value of x. One way out of this difficulty is to multiply the ground state density $P_0^A(k, x)$ with a polynomial so chosen as to make the density function vanish at the nodes. The density for the first excited state, for example, can be taken as

$$P_1^A(k,x) \sim x^2 P_0^A(k,x). \tag{14}$$

Such a choice has been found to work satisfactorily for all the problems considered here. This simple scheme, however, does not work for the second and higher excited states if we do not know the nodal positions exactly. For instance, if we take

$$P_2^A(k,x) \sim (1 - \nu x^2) P_0^A(k,x) \tag{15}$$

for the second excited state and allow variational freedom to all the parameters, $P_2^A(k, x)$ collapses to $P_0^A(k, x)$ corresponding to $\nu = 0$. There is thus the need for a more robust and systematic approach for dealing with excited states. We adopt the following strategy for constructing the excited state densities.

(i) We take $S^A(k, x)$ in (13) to render the trial $P_0^A(k, x)$ reasonably good. We now treat it as a weight function and generate a set of N polynomials in x^2 that form an orthogonal set with respect to this weight function. All these polynomials Q_l have leading coefficient 1. The algorithm below [12,17] can be used to generate these polynomials :

Set $Q_0(x^2) = 1$ and calculate

$$R_0 = \langle Q_0, Q_0 \rangle = \int Q_0(x^2) Q_0(x^2) P_0^A(k,x)\, dx. \tag{16}$$

Next, set

$$Q_1(x^2) = (x^2 - B_0) Q_0(x^2), \tag{17}$$

$$B_0 = \langle x^2 Q_0(x^2), Q_0(x^2) \rangle / R_0. \tag{18}$$

Having obtained $Q_0(x^2)$, ..., $Q_l(x^2)$, one can now evaluate

$$R_l = \langle Q_l(x^2), Q_l(x^2) \rangle; \quad B_l = \langle x^2 Q_l(x^2), Q_l(x^2) \rangle / R_l;$$
$$C_l = R_l / R_{l-1}. \tag{19}$$

The polynomial $Q_{l+1}(x^2)$ is then obtained by exploiting the three-term recurrence relation

$$Q_{l+1}(x^2) = (x^2 - B_l) Q_l(x^2) - C_l Q_{l-1}(x^2) \tag{20}$$

with $Q_{-1} = 0$.

(ii) We form a linear combination of such orthogonal functions within the specified manifold, fix the nonlinear parameters and optimize the linear ones variationally. Such a coupled variational approach ensures high accuracy for at least the first N/2 states [18]. To this end, we construct the Hamiltonian matrix with these set of functions as basis functions and find the excited-state energies by diagonalizing the matrix. It should be pointed out that this variational scheme offers densities of various states as linear combinations of certain basis functions *each* of which obeys the *correct asymptotic behaviour*. We present results for a few even states labelled by the index n in Table 3. Just 15 basis functions have been employed here to construct the

Table 3. Energies of ground ($n = 0$) and even excited states for the potential form (8) *via* the improved VMEP

$V(x)$				Density parameters			n	Energies E_n
α	β	γ	δ	r	t	u		
0	1	0	0	2	1	1/2	0	1.06036209048418
								(1.06036209048418)[a]
							2	7.45569793798677
								(7.45569793798674)[a]
							4	16.2618260188559
								(16.2618260188502)[a]
							6	26.5284711844325
								(26.5284711836825)[a]
							8	37.9230010773345
								(37.9230010270340)[a]
0	40000	0	0	2	1	1/2	0	36.2638733899154
								(36.2638733899154)[a]
							2	254.981282792888
								(254.981282792887)[a]
							4	556.146626825698
								(556.146626825505)[a]
							6	907.260952549708
								(907.260952524100)[a]
							8	1296.94839336072
								(1296.94839164047)[a]
0	0	1	0	3	1	1	0	1.14480245379705
								(1.14480245379705)[a]
							2	9.07308456092145
								(9.07308456092143)[a]
							4	21.7141654222018
								(21.7141654221967)[a]
							6	37.6130865618979
								(37.6130865608952)[a]
							8	56.1993009007144
								(56.1993008525004)[a]
0	0	0	1	3	1	1/2	0	1.225820113800050
								(1.225820113800049)[a]
							2	10.2449469772368
								(10.2449469772369)[a]
							4	25.8090067512976
								(25.8090067512979)[a]
							6	46.3127704950524
								(46.3127704950353)[a]
							8	71.0392576893412
								(71.0392576758820)[a]

[a]See Ref. [10]

Hamiltonian matrix. We happily note that in all cases the energies of the first few excited states are reproduced with almost full machine precision. Here we have additionally considered the x^8 potential for the sake of completeness. Needless to mention, a similar procedure using odd polynomials in x would have led to the PD for odd states.

4. VMEP approach for finite range potentials

It is curious to note that while the MEP has been successfully employed to a wide variety of problems, its applicability to the simplest quantum mechanical system, *viz.* the PB, has not been tested, to the best of our knowledge. The reason is that the MEP ansatz for density fails to satisfy the boundary behaviour as we already pointed out. Hence, in this section, we turn our attention to the ground and excited states of finite range potentials. Here we examine how the form (3) for density can be modulated to simulate the densities of ground and excited states of a few very simple systems. We first consider the PB potential where

$$V(x) = 0, \quad -1 \le x \le 1$$
$$= \infty, \quad |x| > 1 \tag{21}$$

The primitive MEP ansatz with any finite set of λ's cannot ensure the vanishing of $P^1(k, x)$ at $x = \pm 1$. In our VMEP approach we incorporate this behaviour through a *prefactor* of the form $(1-x^2)^\sigma$. For the ground state we thus choose

$$P_0^A(k,x) = (1-x^2)^\sigma \exp\left[-S^A(k,x)\right], \tag{22}$$

$$S^A(k,x) = \sum_{n=1}^{k} \lambda_{2n} x^{2n}. \tag{23}$$

Let us note that here the large-x behaviour poses no problem and hence a few terms of the series representation for $S^1(k, x)$ will suffice. The coefficients λ_{2n} in (23) are treated variationally while the exponent σ is considered to be an adjustable parameter. In Table 4, we show the results of our computation with just *three* parameters in $S^1(k, x)$. The value of σ is restricted to be greater than or equal to 2. This is because, for $\sigma < 2$, the kinetic energy integral *diverges*. The important point to be noted here is the *very sensitive* dependence of the ground state energy on the exponent σ. This clearly shows the adequacy of the modified form (22) for the PD employed by us. Unlike the cases considered earlier, the PB problem is exactly solvable. So here it will be of interest to compare the exact information entropy with that calculated by using the energy-optimized density for various values of σ. This surely provides an additional test of goodness of our modified PD. Table 4 displays the relevant results. The tabulated values clearly justify the workability of our scheme.

Table 4. VMEP results for ground state of PB with $P_0^A(k,x)$ given by (22)

	Ground state energy	Entropy
6 0	2.5808	0.367
4 0	2.5178	0.373
3 0	2.4866	0.378
2 5	2.4801	0.383
2 1	2.4689	0.385
2 01	2.4675	0.3862
2.001	2.46741	0.386285
2.0001	2.467402	0.3862936
2 0	2.467401100274	0.3862944
	(2.467401100272)[a]	(0.3862944)[a]

[a]Exact result

Now we study the excited states by adopting a procedure similar to the one discussed in the previous section. These results are displayed in Table 5. We have chosen here

Table 5. VMEP results for the energies of a few even states of PB

n	E_n	Exact results
	2.467401100272340	2.467401100272340
	22.20660990245097	22.20660990245097
	61.68502750680825	61.68502750680825
	120.9026539133442	120.9026539133442
	199.8594891220587	199.8594891220587

$\sigma = 2.0$ that has emerged out of the calculations just discussed, and 10 basis functions. The accuracy is very good for the lower states. If we want similar accuracy for the higher states we have to routinely increase the number of bases. Since this problem is exactly solvable, one may check how the true density decays to zero at the extremities and compare it with the behaviour of the optimized density that we obtain. Here, it may be verified that the matching is *exact*.

In the case of PB, the potential rises to infinity abruptly at $x = \pm 1$ and the exponent σ in the PD can take only values equal to or greater than 2.0. So it will now be of interest to study another finite-range potential where the exponent can be varied on *either side* of the optimum value. We may also insist that the potential grows to infinity rather softly so that any role of the end effects may become transparent. For this purpose, we have treated the potential

$$(x) = (\pi^2/2)\sec^2(\pi x/2) \tag{24}$$

which is the well-known supersymmetric (SUSY) partner [19, 20] of the PB. Using a PD with the same form as in (22), we get the results displayed in Table 6. We again find that the energy depends sensitively on the value of σ. We also find that the optimum value of σ (= 4.0) comes out to be the same as the one obtained by exact analytical treatment.

Table 6. VMEP results for ground state of SUSY partner of PB given by eq. (24).

σ	Ground state energy	Entropy
5.0	9.8700	0.15151
4.1	9.869609	0.15157
4.01	9.86960444	0.1515733
4.001	9.8696044015	0.1514733
4.0001	9.869604401091	0.1515733
4.0	9.869604401091	0.1515733
3.9999	9.869604401099	0.1515733
3.999	9.8696044016	0.1515733
3.99	9.86960444	0.1515732
3.9	9.869609	0.15157
3.0	9.8701	0.15146
	(9.869604401089)[a]	(0.1515733)[a]

[a] Exact result

It is further noted that though here the ground state energy depends sensitively on the value of σ, the dependence is not as sharp as in the case of the PB. In other words, $(\partial E/\partial\sigma)$ for PB is much larger than the same for its SUSY partner. This difference in behaviour has its origin in the manner in which the potentials approach infinity at the boundaries. The softer the rise of the potential, the less sensitive becomes the dependence of E on σ. Calculations of the information entropy also show a trend similar to that found in the earlier case. Results for the excited states corresponding to the above SUSY partner potential are not separately shown here for brevity. We have, however, checked that the accuracy in this case is as good as in the PB situation.

5. Conclusion

To summarize, our motivation has primarily been to explore how one should employ the MEP form of the PD to gain advantage in studies involving bound quantum states. We hope to have achieved the end. It is quite comforting to note that the whole of the above study bypasses the need to know the exact or approximate value of even a single moment. Thus, we radically depart from traditional implementation of the MEP. Further, a modified form of the MEP ansatz for PD has been shown to be crucial in ensuring the success of the technique. This modification takes account of known small- and large-x behaviours of $P(x)$. We have also overcome the problem of incorporating nodes in $P(x)$ by having recourse to a linear variational strategy in the absence of any other suitable prevalent one. On the other hand, in finite intervals, there is no standard prescription associated with the MEP approach even for the ground state. In this case, we have found that a suitable prefactor that makes the density vanish at either of the boundaries can handle the situation quite commendably. It has also been studied how the nature of the potential dictates the sensitivity of the energy on the form of the prefactor. Additionally, the improved VMEP approach that we have adopted here seems to be highly rewarding from a computational standpoint also. In variational calculations, proper choice of a trial function is crucial. But, there exists nothing like a 'standard choice'. Our pilot calculations indicate that one may use the MEP form of density, with necessary modifications, as a *first* natural choice. Then a linear variational framework may be adopted, in the manner we sketched, to extract still more accurate results for both ground and excited states.

Extension of the above formalism to multidimensional problems with *separable* potentials is straightforward. Atomic problems under a central-field approximation can also be treated *via* the scheme outlined here. In this context, we may also mention that the application of information entropy to the Thomas-Fermi model of atoms has been successfully pursued (see, *e.g.* [21] and references therein). However, for nonseparable potentials, a simple ansatz for the density like (3) cannot be obtained. Indeed, any moment-based approach

is likely to encounter difficulties in such situations [22]. Finally, the 'entropy' considered in this and related works refers not to the randomness in energy space, but to the entropy of the distribution in position space corresponding to pure states. The latter quantity obviously possesses a nonzero value.

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